Superfluid-Mott-Insulator Transition in a One-Dimensional Optical Lattice with Double-Well Potentials

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(Dated: February 6, 2008)

We study the superfluid-Mott-insulator transition of ultracold bosonic atoms in a one-dimensional optical lattice with a double-well confining trap using the density-matrix renormalization group. At low density, the system behaves similarly as two separated ones inside harmonic traps. At high density, however, interesting features appear as the consequence of the quantum tunneling between the two wells and the competition between the "superfluid" and Mott regions. They are characterized by a rich step-plateau structure in the visibility and the satellite peaks in the momentum distribution function as a function of the on-site repulsion. These novel properties shed light on the understanding of the phase coherence between two coupled condensates and the off-diagonal correlations between the two wells.

I. INTRODUCTION

The experimental realization of trapped ultracold bosonic gases on optical lattices has opened up the possibility of observing various quantum phases (e.g., superfluid and Mott insulator) and studying the quantum phase transitions between them in a well-controlled manner. Without the confining trap, the system will undergo a superfluid-Mott-insulator phase transition at integer fillings. In the presence of a confining trap, the superfluid and Mott-insulator regions may coexist[1,2] due to the inhomogeneity induced by the trap.

Numerical calculations have been carried out for the systems without[3,4] and with a harmonic trap[5,6,7,8], using the quantum Monte Carlo and density-matrix renormalization group[9,10] (DMRG) methods. Interesting new features appear in the system with a single harmonic confining trap, which are associated with the competition between the "superfluid" and Mott insulator regimes and characterized by the "kinks"[7] in the visibility of interference fringes with the increase of the on-site repulsion.

Recently a bosonic Josephson junction composed of two weakly coupled Bose-Einstein condensates in a macroscopic double-well potential has been experimentally realized[11]. It raises an interesting question concerning the quantum tunnelling effect in a double-well potential system in which the ultracold atoms on optical lattice are trapped. In such a system, the inter-atom interaction and the competition between the "superfluidity" and Mott insulator phases are expected to play a crucial role in shaping the inter-well tunnelling.

In this paper, we intend to clarify this issue by studying a one-dimensional Bose-Hubbard model in the presence of a double-well potential using the DMRG. At low filling ($\rho = 1/2$), we find the system simply behaves as two separated ones, each of which is in a harmonic trap without significant coupling between them. At a higher filling ($\rho = 1$), however, the bosons in the two wells become

strongly correlated and a rich phenomenon related to the evolution of the "superfluid" and Mott insulator regions as a function of the on-site repulsion is obtained. A detailed discussion on how to detect these features based on the visibility, momentum distribution, hopping correlation function, and other physical quantities is given. These novel properties shed light on the understanding of the phase coherence and off-diagonal correlation between the coupled condensates in a double-well interacting Bose system on optical lattices.

A cold atomic Bose gas on a one-dimensional optical lattice in the presence of a double-well potential trap can be described by the following Bose-Hubbard Hamiltonian

$$
\begin{aligned}
H = & -t\sum_i \left(\hat{a}_i^\dagger \hat{a}_{i+1} + h.c. \right) \\
& +U\sum_i \hat{n}_i(\hat{n}_i - 1)/2 + \sum_i V_T(i)\hat{n}_i,
\end{aligned} \tag{1}
$$

where

$$
V_T(i) = V_{T1}\left(i - \frac{L+1}{2} \right)^2 + V_{T2}\left(i - \frac{L+1}{2} \right)^4 \tag{2}
$$

is the double-well trap with quadratic V_{T1} and quartic V_{T2} coefficients, and L is the number of sites. The hopping integral t is set as the unit of energy $t = 1$, and U is the on-site repulsion. $\hat{a}_i^\dagger$ and $\hat{a}_i$ are the bosonic creation and annihilation operators, respectively, and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the number operator.

An important parameter in characterizing the phase coherence in a superfluid-Mott-insulator transition is the visibility of interference fringes defined by[12,13]

$$
\nu = \frac{S_{\max} - S_{\min}}{S_{\max} + S_{\min}}, \tag{3}
$$

where $S_{\max}$ and $S_{\min}$ are the maximum and minimum of the momentum distribution function

$$
S(\mathbf{k}) = \frac{1}{L}\sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \left\langle \hat{a}_i^\dagger \hat{a}_j \right\rangle. \tag{4}
$$

In the presence of a confining trap, it is useful to introduce the local density of bosons $n_i = <\hat{n}_i>$ and the local particle fluctuation[6]

$$\kappa_i \equiv [\langle \hat{n}_i^2 \rangle - n_i^2], \qquad (5)$$

to measure the inhomogeneity induced by the confining trap. To further quantify the spatial correlations within the trap potential, we have also calculated the hopping correlation function

$$g(i,j) = \left\langle \hat{a}_i^\dagger \hat{a}_j \right\rangle \qquad (6)$$

between two lattice sites i and j, the total interaction energy E_U,

$$E_U = U \sum_i n_i (n_i - 1)/2, \qquad (7)$$

the kinetic energy $|E_k|$,

$$E_k = -t \sum_i \left\langle \hat{a}_i^\dagger \hat{a}_{i+1} + h.c. \right\rangle, \qquad (8)$$

and the trapping energy E_T

$$E_T = \sum_i V_T(i) n_i, \qquad (9)$$

respectively.

II. SUPERFLUID-MOTT-INSULATOR TRANSITION

In the following we present our DMRG calculations for the Bose-Hubbard model (1). Compared with a harmonic trap[7], the present system shows a richer and more complex structure, due to the coupling between the two wells. When the density is low enough such that there is no particle in the middle of the system, the system splits into two weakly coupled harmonic ones. However, if the density is sufficiently high that particles in the two wells are not well separated, the interaction between the wells will play a crucial role, which may change the behavior of the system dramatically.

In the following, we will consider the system with 80 sites in a double-well trap potential with $V_{T1} = -0.024t$ and $V_{T2} = 2 \times 10^{-5}t$. The calculations are carried out using the DMRG with open boundary conditions, for two different filling factors $\rho = 1/2$ and $\rho = 1$.

A. Filling $\rho = 1/2$

AT the filling $\rho = 1/2$, the system will not reach a Mott-insulator state, even in the Tonks-Girardeau (TG) limit $U \to \infty$, without a trap potential V_T. In the presence of the double-well potential, however, two separated Mott-insulator domains with the density $n_i = 1$ appear
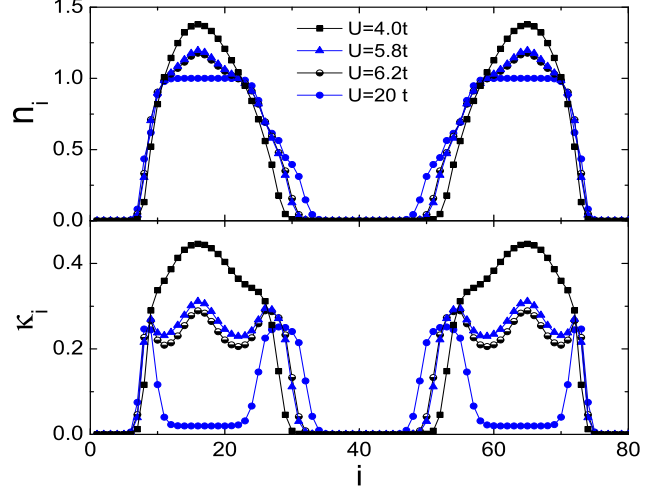

FIG. 1: Density profiles n_i and the corresponding particle fluctuation κ_i for $\rho = 1/2$. The profiles for $U = 5.8t$ and $U = 6.2t$ nearly coincide.

inside the two wells at large U, due to the low density of the system. Fig. 1 shows the density profile and corresponding particle fluctuation at various values of U/t. At small U/t, two separate superfluid regions appear in the two wells. When U is increased, the superfluid regions shrink until the Mott-insulator domains emerge when U/t is larger than 6.8.

To further quantify this transition, let us define the integrated density

$$N_d = \sum_{i=l_1}^{l_2} n_i \qquad (10)$$

in a range $[l_1, l_2]$. In the present system, we choose $l_1 = 11$ and $l_2 = 22$ in the left-side well. As shown in Fig.2 (a), N_d is saturated to a plateau of $N_d = 12$ corresponding to a local Mott-insulator state $(n_i = 1)$ as U/t is increased beyond 6.8.

Fig.2(a) shows the visibility ν. Two kinks can be observed. The first one (less evident) occurs around $U/t = 5.5$, while the second one around $U/t = 6.4$. As U/t is increased between 5.8 and 6.2, there is almost no change in the density profile. This is due to presence of the emergent Mott-insulator regions surrounding the superfluid ones in the two wells. The atoms in the central superfluid regions can transfer to the outer superfluid regions at larger U/t. This will eventually exhaust the superfluid regions in the two well centers. At $U/t = 20$, the flat Mott-insulator plateaus, with vanishing local particle fluctuation, centered around the two wells are clearly seen.

As shown in Fig. 2, the visibility with the corresponding E_T, E_U and the ratio $\gamma = |E_U/E_k|$, exhibits a characteristic kink structure. The quick decrease of E_U in
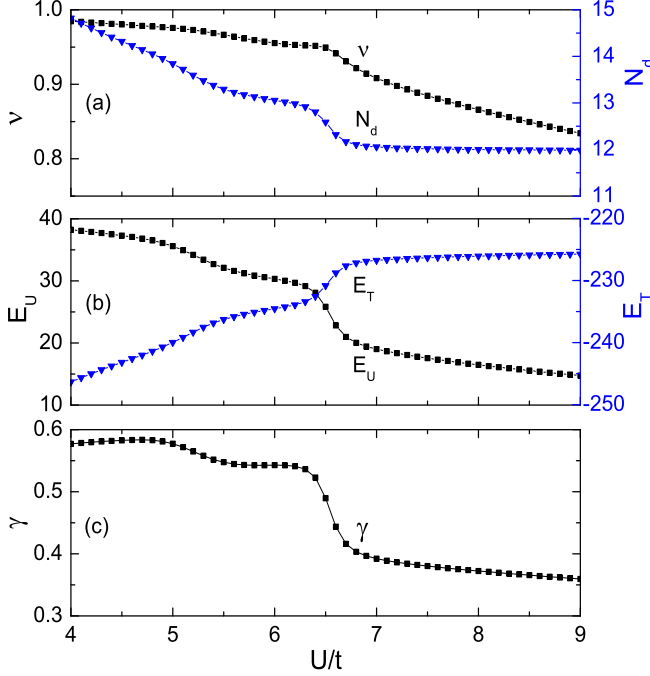
FIG. 2: (a) Visibility ν and integrated density N_d; (b) Interaction energy E_U and trapping energy E_T; (c) Ratio $\gamma = |E_U/E_k|$ of interaction to kinetic energy, as functions of U/t, for the filling factor $\rho = 1/2$.
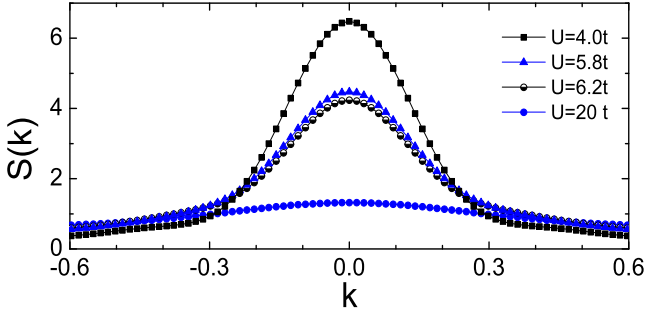

FIG. 4: (a) Visibility ν and integrated density N_d from $l_1 = 11$ to $l_2 = 30$, (b) Kinetic $|E_k|$ and total energy E_S, (c) Ratio $\gamma = |E_U/E_k|$ of interaction to kinetic energy, as functions of U/t for $\rho = 1$.

FIG. 3: Momentum distribution function $S(k)$ for the system shown in Fig. 1.

the interval $U/t = 6.2 - 6.8$ shows a great suppression of the double occupancy in the two wells. It is a manifestation of the transition from superfluid to Mott-insulator in the two wells. This occurs even though the total energy increases continuously with the increase of U/t. By further increasing U/t, the density profile remains almost unchanged.

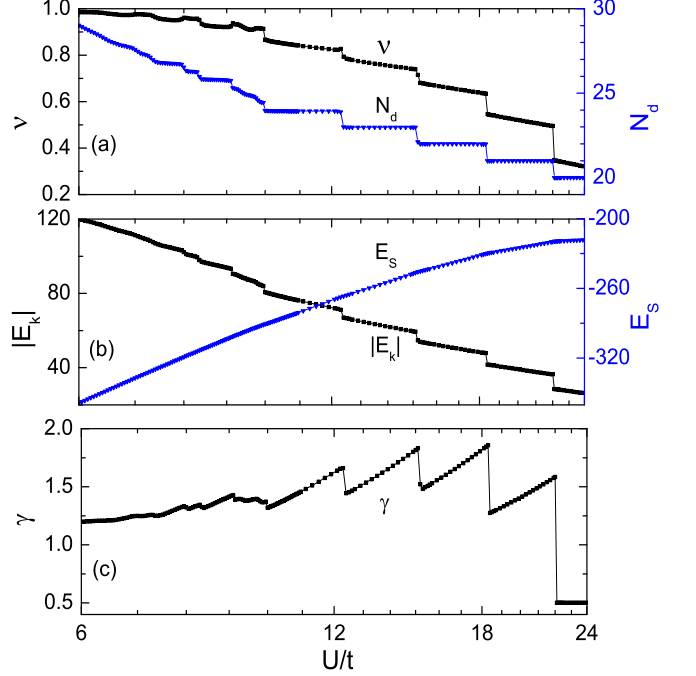Fig. 3 shows the corresponding momentum distribu-

tion function $S(k)$ for the system shown in Fig.1. When U/t is small, the system is in a superfluid state and a single narrow peak appears at zero momentum in $S(k)$. For large U/t, $S(k)$ is broadened. The quantitative change in $S(k)$ is best reflected in the kink structure of the visibility ν. In he Tonks-Girardeau limit, we find that $S_{\max} = 1.04$ and $\nu = 0.44$. The non-zero visibility ν reveals the presence of the superfluid regions surrounding the Mott-insulator plateau regions (Fig. 1).

Finally, we note that at $\rho = 1/2$, the distribution of bosons remains well separated in the two wells [Fig.1]. Therefore, it can be approximately treated as two single wells with weak coupling. Indeed, the results presented above are consistent with those obtained in a harmonic trap[7].

B. Filling $\rho = 1$

At $\rho = 1$, bosons inside the two wells cannot be separated for sufficiently large U. The system is in a Mott-insulator state without the trap in the TG limit.

Fig.4(a) shows the visibility ν and the integrated density N_d ($l_1 = 11$, $l_2 = 30$) defined in Eq.(10). The evolution of these two quantities exhibit a rich step-plateau structure compared with the case of $\rho = 1/2$. When U is
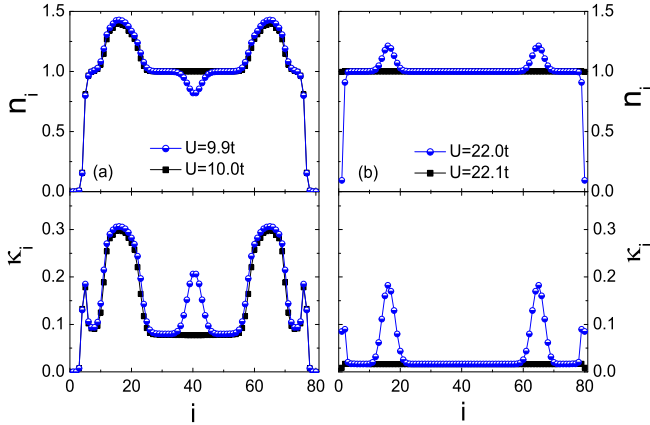
FIG. 5: Density profiles n_i and the corresponding local particle fluctuation κ_i for $\rho = 1$.

small (about $\leq 10t$), the central Mott-insulator domain has not formed. In this parameter regime, the plateaus in ν and N_d are quite narrow, indicating that the Mott-insulator domains surrounding the superfluid ones are not robust and the bosons can escape from the superfluid regions in the two wells. This feature is well reflected in the density profiles and local particle fluctuation around the step between $U/t = 9.9$ and 10 as shown in Fig.5(a).

When U/t is further increased, the central region of the system shows a flat Mott-insulator plateau with $n_i = 1$ [Fig. 5]. This leads to a sudden decrease in ν and N_d. Due to the large on-site repulsion U and the existence of the central Mott-insulator regions, bosons can only tunnel from the inner superfluid region to the outer ones. Whenever a boson escapes from the superfluid region, the visibility ν as well as the integrated density N_d shows a sharp decrease. When U/t is larger than 22, the superfluid region disappears competely (Fig.5(b)). In the TG limit, the whole system is in a Mott-insulator state and $\kappa_i = 0$.

As shown in Fig. 4(b), the abrupt changes are also present in $|E_k|$ at the steps of ν, although the total energy E_S increases smoothly with U/t. The steps in $|E_k|$ can be understood as the abrupt redistribution of the boson density between the superfluid and Mott-insulator regions. During this process, the superfluid region becomes smaller, while the Mott-insulator becomes larger. The monotonic decrease of $|E_k|$ with increasing U/t is due to the widening of the Mott insulator regions in which the kinetic energy is suppressed. In the plateau regions, the increase in γ is also due to the reduction of the kinetic energy.

Fig. 6 shows the momentum distribution function $S(k)$. $S(k)$ exhibits different features at different U/t regimes. Furthermore, $S(k)$ is correlated with ν. When the satellite peaks appear in $S(k)$, ν undergoes a sharp increase; while ν undergoes a sharp decrease when the
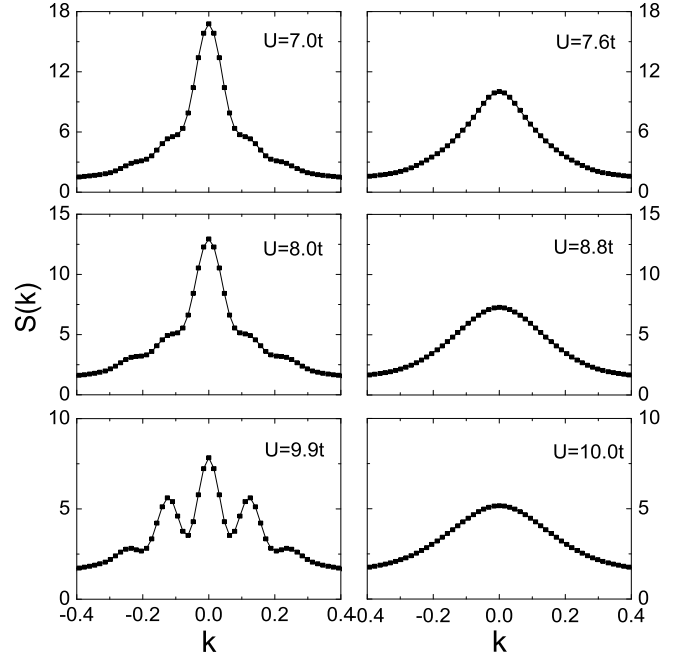

FIG. 6: Momentum distribution function $S(k)$ at different values of U/t for $\rho = 1$.

satellite peaks disappear.

More detailed study demonstrates that the satellite peak structure in $S(k)$ is related to the existence of a strong off-diagonal long-range correlation between the two wells. This can be seen from Fig. 7, in which the hoping correlation function $g(16, i)$ between site 16 and site i is plotted. If the system has an off-diagonal long-range correlation, the satellite peaks are present in $S(k)$. If the system does not have the off-diagonal long-range correlation, the satellite peaks disappear. These features are different from those in a harmonic trap[5]. All the above features appear before the formation of the central Mott-insulator plateau. In the presence of the central Mott-insulator plateau, however, the satellite structure of $S(k)$ as well as the long-range off-diagonal correlation between the two wells disappears. This suggests that one can judge whether or not the off-diagonal long-range correlation exists from the measurement of momentum distribution functions.

III.   SUMMARY

To summarize, we have explored the superfluid-Mott-insulator transition in a double-well trapped atomic Bose gas in a one-dimensional optical lattice using the DMRG. We find that this transition is well characterized by the visibility ν, which exhibits a series of kink structures associated with the redistribution of bosons between local
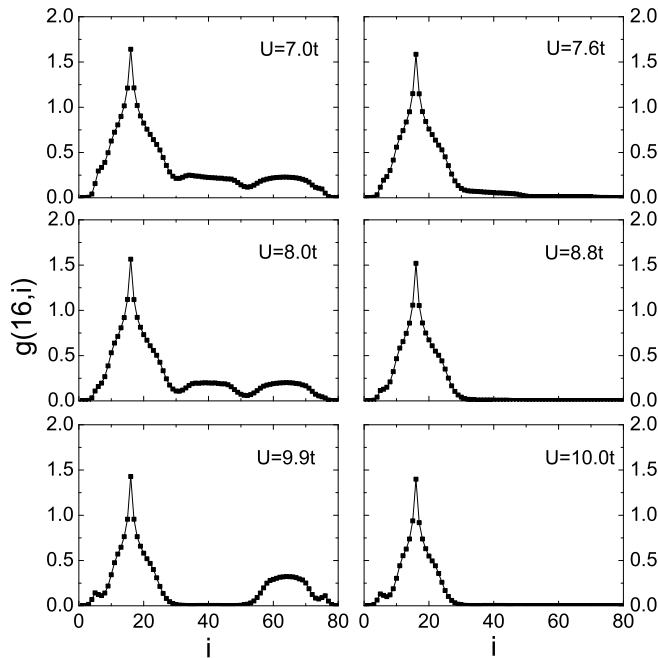
FIG. 7: Hopping correlation function $g(16,i)$ between site 16 and i at different values of U/t for $\rho = 1$.

superfluid and Mott-insulator regions, as a function of the on-site repulsion U. The evolution of the system also shows a number of characteristic features in the local integrated density, the density profile, local compressibility, and the momentum distribution.

At low density (e.g. $\rho = 1/2$), the system behaves like two weakly coupled harmonic traps. With the increase of the density, the system begins to develop novel properties unique to the double well potential associated with a strong quantum tunneling effect between the two wells. At high density (e.g. $\rho = 1$), a series of steps and plateaus appear in the visibility and other physical quantities. These features are related to the abrupt redistribution of the bosons in the local superfluid and Mott-insulator regions. In addition, the presence of the satellite peaks in the momentum distribution function indicates that the strong off-diagonal long-range correlation between the superfluid regions are separated by the Mott insulator regions. Therefore, it is an effective probe for experiment to identify the off-diagonal long-range correlation and phase coherence due to the tunnelling between the two condensates on the optical lattice.

IV. ACKNOWLEDGEMENT

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